

Output

Axes	K(TPa ⁻¹)	σK (TPa ⁻¹)	Direction			Empirical parameters			P_c	ν
			a	b	c	ϵ_0	λ			
X_1	8.1372	0.0849	1.0000	-0.0000	-0.0000	-4.1800e-04	-7.3876e-03		0.0000	1.0869
X_2	8.1372	0.0849	0.0000	1.0000	-0.0000	-4.1800e-04	-7.3876e-03		0.0000	1.0869
X_3	8.1372	0.0849	0.0000	0.0000	1.0000	-4.1800e-04	-7.3876e-03		0.0000	1.0869
V	23.6288	0.2177								

Birch-Murnaghan Coefficients

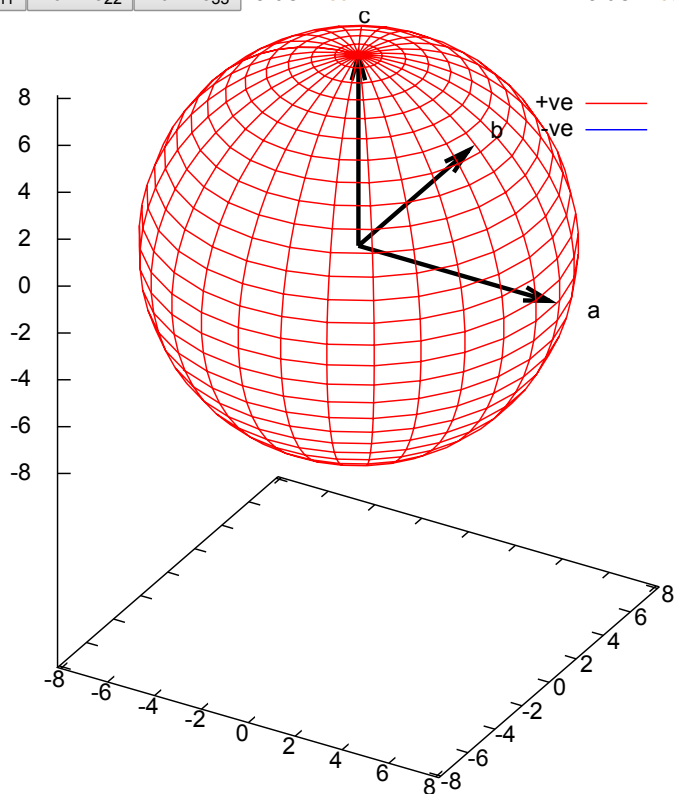
	B_0 (GPa)	σB_0 (GPa)	V_0 (Å ³)	σV_0 (Å ³)	B'	$\sigma B'$	P_c (GPa)
2 nd	37.0122	0.6353	14930.7970	7.6752	4	n/a	0
3 rd	45.7903	1.2122	14904.3916	4.4478	-3.3283	0.8571	0

Compressibility Indicatrix

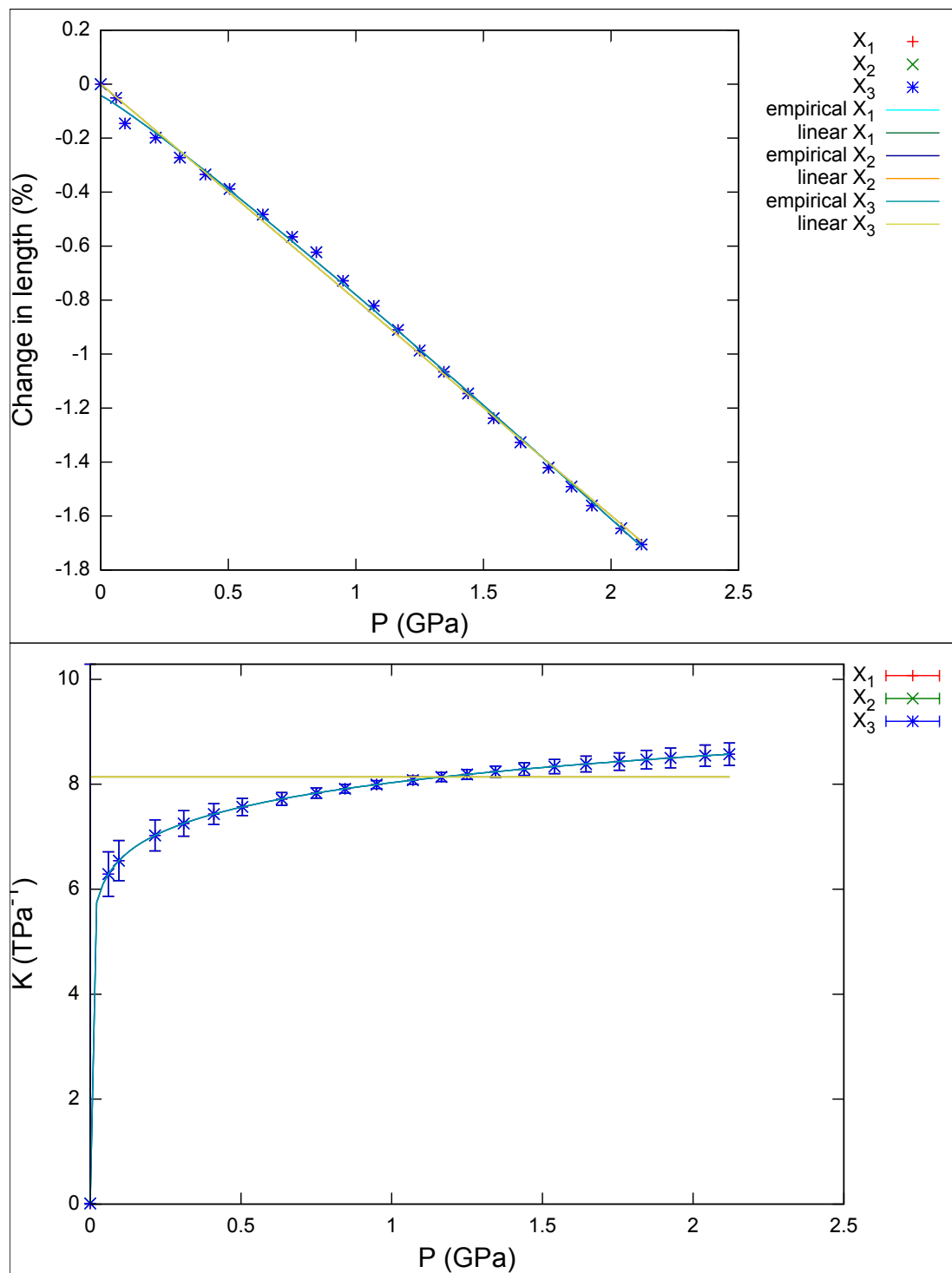
The compressibility indicatrix has units of TPa⁻¹.

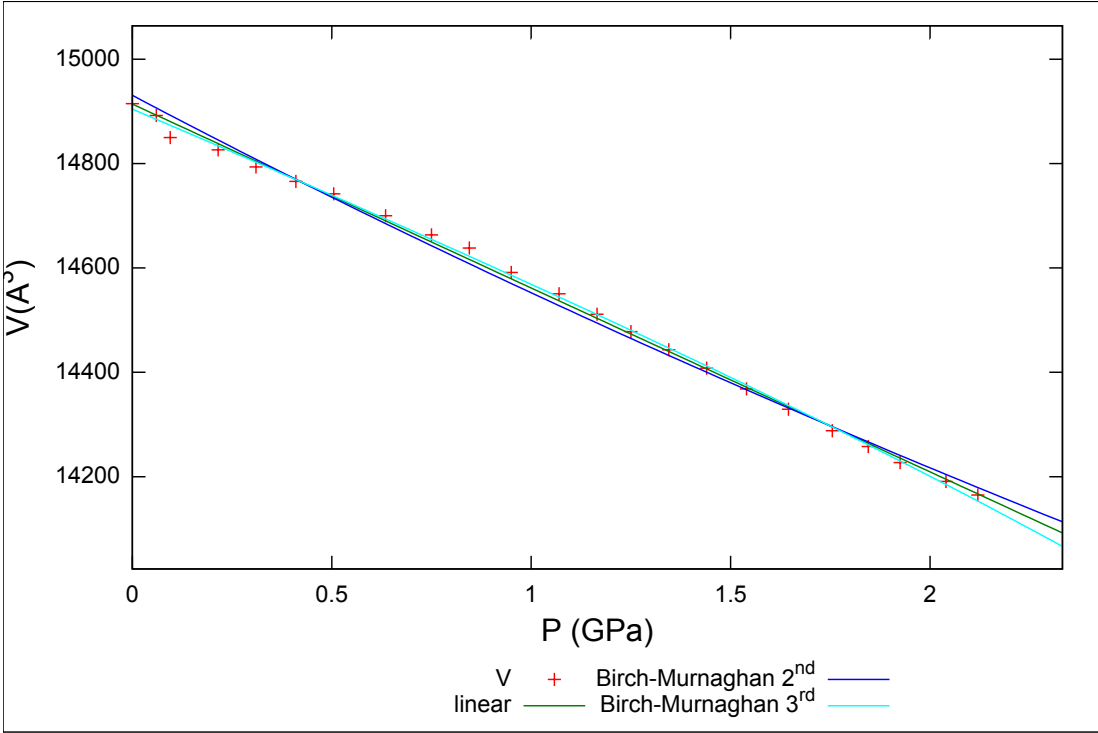
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down e_{11}	Down e_{22}	Down e_{33}	Value X:30

Value Z:60



Plots





Compressibilities (TPa⁻¹)

P	K ₁	K ₂	K ₃	σK ₁	σK ₂	σK ₃
0.00	0.01	0.01	0.01	6067493294959447046812073984.00	6067493294959447046812073984.00	6067479715341742925708001280.00
0.06	6.29	6.29	6.29	0.42	0.42	0.42
0.10	6.54	6.54	6.54	0.38	0.38	0.38
0.21	7.03	7.03	7.03	0.30	0.30	0.30
0.31	7.25	7.25	7.25	0.24	0.24	0.24
0.41	7.43	7.43	7.43	0.20	0.20	0.20
0.51	7.57	7.57	7.57	0.16	0.16	0.16
0.64	7.72	7.72	7.72	0.12	0.12	0.12
0.75	7.83	7.83	7.83	0.10	0.10	0.10
0.84	7.91	7.91	7.91	0.08	0.08	0.08
0.95	7.99	7.99	7.99	0.07	0.07	0.07
1.07	8.08	8.08	8.08	0.08	0.08	0.08
1.17	8.14	8.14	8.14	0.08	0.08	0.08
1.25	8.19	8.19	8.19	0.09	0.09	0.09
1.34	8.24	8.24	8.24	0.11	0.11	0.11
1.44	8.29	8.29	8.29	0.12	0.12	0.12
1.54	8.34	8.34	8.34	0.13	0.13	0.13
1.65	8.38	8.38	8.38	0.15	0.15	0.15
1.75	8.43	8.43	8.43	0.17	0.17	0.17
1.84	8.47	8.47	8.47	0.18	0.18	0.18
1.93	8.50	8.50	8.50	0.19	0.19	0.19
2.04	8.54	8.54	8.54	0.20	0.20	0.20
2.12	8.57	8.57	8.57	0.21	0.21	0.21

% change in length

P	X ₁	X ₂	X ₃	X _{1,calc}	X _{2,calc}	X _{3,calc}
0.0000	0.0000	0.0000	0.0000	-0.0418	-0.0418	-0.0418
0.0600	-0.0510	-0.0510	-0.0510	-0.0765	-0.0765	-0.0765
0.0950	-0.1460	-0.1460	-0.1460	-0.0990	-0.0990	-0.0990
0.2150	-0.1982	-0.1982	-0.1982	-0.1808	-0.1808	-0.1808
0.3100	-0.2720	-0.2720	-0.2720	-0.2486	-0.2486	-0.2486
0.4100	-0.3346	-0.3346	-0.3346	-0.3221	-0.3221	-0.3221
0.5050	-0.3882	-0.3882	-0.3882	-0.3934	-0.3934	-0.3934
0.6350	-0.4830	-0.4830	-0.4830	-0.4927	-0.4927	-0.4927
0.7500	-0.5657	-0.5657	-0.5657	-0.5822	-0.5822	-0.5822
0.8450	-0.6227	-0.6227	-0.6227	-0.6570	-0.6570	-0.6570
0.9500	-0.7285	-0.7285	-0.7285	-0.7405	-0.7405	-0.7405

1.0700 -0.8214 -0.8214 -0.8214 -0.8369 -0.8369 -0.8369
 1.1650 -0.9106 -0.9106 -0.9106 -0.9140 -0.9140 -0.9140
 1.2500 -0.9866 -0.9866 -0.9866 -0.9833 -0.9833 -0.9833
 1.3450 -1.0656 -1.0656 -1.0656 -1.0614 -1.0614 -1.0614
 1.4400 -1.1462 -1.1462 -1.1462 -1.1399 -1.1399 -1.1399
 1.5400 -1.2375 -1.2375 -1.2375 -1.2230 -1.2230 -1.2230
 1.6450 -1.3269 -1.3269 -1.3269 -1.3108 -1.3108 -1.3108
 1.7550 -1.4211 -1.4211 -1.4211 -1.4033 -1.4033 -1.4033
 1.8450 -1.4908 -1.4908 -1.4908 -1.4794 -1.4794 -1.4794
 1.9250 -1.5615 -1.5615 -1.5615 -1.5472 -1.5472 -1.5472
 2.0400 -1.6455 -1.6455 -1.6455 -1.6452 -1.6452 -1.6452
 2.1200 -1.7056 -1.7056 -1.7056 -1.7137 -1.7137 -1.7137

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.0000	-0.0028	0.0392	-0.0327	14915.0155
0.0600	0.0620	0.0963	0.0374	14892.2051
0.0950	0.1823	0.2036	0.1670	14849.7841
0.2150	0.2484	0.2631	0.2377	14826.5171
0.3100	0.3416	0.3479	0.3371	14793.6488
0.4100	0.4206	0.4205	0.4208	14765.8140
0.5050	0.4882	0.4831	0.4921	14741.9963
0.6350	0.6075	0.5950	0.6171	14699.9511
0.7500	0.7114	0.6937	0.7251	14663.3231
0.8450	0.7830	0.7624	0.7989	14638.1060
0.9500	0.9155	0.8911	0.9345	14591.4089
1.0700	1.0316	1.0056	1.0521	14550.4839
1.1650	1.1428	1.1167	1.1636	14511.2863
1.2500	1.2375	1.2125	1.2575	14477.9182
1.3450	1.3358	1.3130	1.3541	14443.2881
1.4400	1.4359	1.4167	1.4514	14407.9974
1.5400	1.5490	1.5354	1.5601	14368.1272
1.6450	1.6596	1.6529	1.6650	14329.1429
1.7550	1.7760	1.7782	1.7738	14288.1465
1.8450	1.8619	1.8719	1.8531	14257.8625
1.9250	1.9490	1.9679	1.9326	14227.1650
2.0400	2.0522	2.0829	2.0254	14190.7836
2.1200	2.1260	2.1659	2.0909	14164.8064

Input

P	σP	a	b	c	α	β	γ
0	0.1	24.615457	24.615457	24.615457	90	90	90
0.06	0.1	24.602902	24.602902	24.602902	90	90	90
0.095	0.1	24.579519	24.579519	24.579519	90	90	90
0.215	0.1	24.566675	24.566675	24.566675	90	90	90
0.31	0.1	24.548508	24.548508	24.548508	90	90	90
0.41	0.1	24.533102	24.533102	24.533102	90	90	90
0.505	0.1	24.519904	24.519904	24.519904	90	90	90
0.635	0.1	24.496571	24.496571	24.496571	90	90	90
0.75	0.1	24.476208	24.476208	24.476208	90	90	90
0.845	0.1	24.462169	24.462169	24.462169	90	90	90
0.95	0.1	24.436129	24.436129	24.436129	90	90	90
1.07	0.1	24.413262	24.413262	24.413262	90	90	90
1.165	0.1	24.39132	24.39132	24.39132	90	90	90
1.25	0.1	24.37261	24.37261	24.37261	90	90	90
1.345	0.1	24.353162	24.353162	24.353162	90	90	90
1.44	0.1	24.333311	24.333311	24.333311	90	90	90
1.54	0.1	24.310845	24.310845	24.310845	90	90	90
1.645	0.1	24.288838	24.288838	24.288838	90	90	90
1.755	0.1	24.265652	24.265652	24.265652	90	90	90
1.845	0.1	24.248496	24.248496	24.248496	90	90	90
1.925	0.1	24.231081	24.231081	24.231081	90	90	90
2.04	0.1	24.210409	24.210409	24.210409	90	90	90

2.12 0.1 24.195627 24.195627 24.195627 90 90 90